Information Content of Infrared Satellite Sounding Measurements with Respect to CO₂

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ABSTRACT

Information theory is used to study the capabilities of the new-generation satellite infrared sounders [Atmospheric Infrared Sounder (AIRS) and Infrared Atmospheric Sounding Interferometer (IASI)] for retrieving atmospheric carbon dioxide ($\rm CO_2$) and for contrasting these new instruments with the current system of infrared sounders [Television and Infrared Observation Satellite (TIROS) Operational Vertical Sounder/High-Resolution Infrared Radiation Sounder (TOVS/HIRS)]. It is shown that instruments like AIRS and IASI will be able to retrieve column-averaged $\rm CO_2$ mixing ratios with high enough accuracy (order of 1–2 ppmv) to be useful for atmospheric $\rm CO_2$ inversion studies that try to estimate sources and sinks of $\rm CO_2$. On the other hand, the TOVS/HIRS system is only able to retrieve column-averaged $\rm CO_2$ mixing ratios with an accuracy of the same order as the seasonal amplitude of atmospheric $\rm CO_2$ variations (order of 10 ppmv). It is also shown that the constraining a priori covariance matrix has an important effect on what information can be extracted from the observations.

1. Introduction

Atmospheric carbon dioxide (CO₂) has increased from about 280 to about 375 ppmv since the beginning of the industrial era. The rate of combustion of fossil fuels is known from econometric tabulations (e.g., Andres et al. 1996), and so the history of atmospheric CO₂ can be used to infer the integral of all other sources and sinks in the earth system by subtracting this anthropogenic emission rate. Surface measurements from a sparse global network indicate the biosphere and oceans have absorbed about one-half of the carbon emitted by fossil fuel consumption during the past 20 yr (e.g., Francey et al. 1995). The geographic distribution of these sinks and the underlying mechanisms that control them, however, are too uncertain to predict how these processes will change future emission uptakes.

A way to deduce the distribution of sources and sinks is to apply measurements of CO₂ in an inversion model that takes into account transport processes (e.g., Enting et al. 1995; Gurney et al. 2002). Until now, the current flask network has been used for this purpose, but the distribution of these measurements is too sparse to provide the necessary coverage for these inversion studies (Engelen et al. 2002). Al-

though the individual flask measurements are of high precision (Masarie and Tans 1995), additional spatially resolved global maps of CO₂, with a precision of about 1 ppmv, offer the potential to improve dramatically our ability to quantify the sources and sinks of CO₂ and the distribution of these fluxes (Rayner and O'Brien 2001).

The study of Rayner and O'Brien (2001) points to the potential value of satellite-based remote sensing methods for studying the carbon cycle. The recent study of Chédin et al. (2002) demonstrates how the seasonal signatures of CO₂ can be observed in Television and Infrared Observation Satellite Operational Vertical Sounder/High-Resolution Infrared Radiation Sounder (TOVS/HIRS) measurements, and the study of Engelen et al. (2001) highlights the potential of the future measurements of the Atmospheric Infrared Sounder (AIRS). The purpose of this paper is to provide further analysis of the capabilities of the nextgeneration sounders, such as AIRS and the Infrared Atmospheric Sounding Interferometer (IASI), and to contrast these capabilities with those of the currentgeneration TOVS/HIRS instruments. We attempt to quantify CO₂ information content contained in these types of infrared measurement systems. The next section outlines the basic information theory used to characterize these observing systems and illustrates the principles with use of a simple example. This theory is applied to HIRS and AIRS-like observations in section 3, where it is shown that the HIRS observations cannot be expected to resolve CO₂ variation below about 10 ppmv, which barely resolves gross

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seasonal swings in CO_2 , whereas AIRS and IASI are expected to resolve mean tropospheric CO_2 mixing ratios below about 1–2 ppmv.

2. Information content

a. Theory

To calculate the information content of infrared satellite radiances with respect to atmospheric CO_2 concentrations, we followed the description by Rodgers (2000), which is based on the definition by Shannon and Weaver (1949). The information content of a set of observations is defined by the change in the logarithm (base 2) of the number of distinct possible states of the system being measured. If we define the possible states of a system with a probability distribution function P and the entropy of this system as S(P), the information content of a set of observations is the change in entropy

$$H = S(P_1) - S(P_2), (1)$$

where P_1 represents our knowledge before the observations are made and P_2 is our knowledge after the observations are made. If we assume Gaussian probability distributions, we can define the entropy as

$$S(P) = \frac{1}{2} \ln|\mathbf{S}|,\tag{2}$$

where **S** is the covariance matrix that describes our knowledge of the system. The entropy can be seen as the logarithm of the volume of state space occupied by the probability density function defined by the covariance matrix. The information content is then

$$H = \frac{1}{2}\ln|\mathbf{S}_1| - \frac{1}{2}\ln|\mathbf{S}_2| = -\frac{1}{2}\ln|\mathbf{S}_2\mathbf{S}_1^{-1}|, \quad (3)$$

with \mathbf{S}_1 being the prior covariance and \mathbf{S}_2 being our posterior covariance. It therefore represents the reduction in volume of the prior probability function by making the observations. This means that of all the possible atmospheric profiles within the atmospheric profile space defined by the a priori covariance matrix, a total of 2^H profiles can actually be distinguished by the observations.

Another useful measure of information is the degrees of freedom for signal. Although the total degrees of freedom of a set of observations is equal to the number of observations, only a selection of these total degrees of freedom is independent and significant with respect to the measurement noise. The degrees of freedom for signal are therefore defined as the number of independent pieces of information in a measurement that can be observed above the noise of the observations. Using the preceding covariance definitions, we can write the degrees of freedom for signal as the trace of the same matrix product as is used in the definition of the Shannon information content $(\mathbf{S}_2\mathbf{S}_1^{-1})$:

TABLE 1. Retrieval error, degrees of freedom for signal, and information content for a simple measurement.

	Small measurement error	Large measurement error
σ_y (ppmv)	0.25	4.0
σ_a (ppmv)	4.0	0.25
$\sigma_{\rm r}$ (ppmv)	0.235	0.235
d_s	0.94	0.06
\ddot{H}	4.09	0.089

$$d_s = \operatorname{tr}(\mathbf{S}_2 \mathbf{S}_1^{-1}). \tag{4}$$

b. A simple flask measurement example

A simple example can show the use of the earlier-defined measures of information in an observation. Assume we want to retrieve the true value of the CO_2 concentration x from a direct flask observation y given some a priori guess of x. If the observation includes an error ε , we have the following relation between x and y:

$$y = x + \varepsilon. (5)$$

We can then calculate the retrieval error given the measurement error and the a priori error from

$$\sigma_{x}^{2} = (\sigma_{a}^{-2} + \sigma_{y}^{-2})^{-1}, \tag{6}$$

where standard deviations are used to represent the errors. The information content and degrees of freedom for signal can then be calculated from (3) and (4), respectively. Table 1 shows the results for two cases: (i) a small-measurement-error case (measurement error is 0.25 ppmv and a priori error is 4 ppmv) and (ii) a large-measurement-error case (measurement error is 4 ppmv and a priori error is 0.25 ppmv).

Although the retrieval error σ_r is the same for both retrievals, the degrees of freedom and the information content are very different. In the case with small measurement error, the degrees of freedom for signal is almost 1; in the case with large measurement error, the degrees of freedom for signal is almost zero. As expected, the information content of the low noise measurement is much larger than the information content of the high noise measurement. The low observational noise retrieval can distinguish $2^4 = 16$ values within the a priori variance of 4 ppmv, which in this scalar case is equal to the signalto-noise ratio defined by σ_a/σ_v . In other words, although the retrieval error does not distinguish between the lowand high-noise cases, the degrees of freedom and the information content differentiate between the two cases and identify the better measurement system.

c. A more general example

In a more realistic environment, such as the retrieval of CO₂ concentrations from infrared satellite observations (Engelen et al. 2001) that we are considering in this paper, a linear relation between the retrieval vari-

ables \mathbf{x} and the observations \mathbf{y} can be constructed such that

$$\mathbf{y} = \mathbf{K}\mathbf{x},\tag{7}$$

where **K** is the weighting function matrix. Using a constraint in the form of an a priori covariance matrix \mathbf{S}_a , we can write the retrieval error covariance matrix as

$$\mathbf{S}_{r} = (\mathbf{S}_{a}^{-1} + \mathbf{K}^{T}\mathbf{S}_{v}^{-1}\mathbf{K})^{-1},$$
 (8)

where \mathbf{S}_y is the measurement error covariance matrix. Because the information content and the degrees of freedom for signal are defined with respect to the a priori covariance matrix and the measurement covariance matrix, we scale the weighting function matrix accordingly:

$$\tilde{\mathbf{K}} = \mathbf{S}_{v}^{-1/2} \mathbf{K} \mathbf{S}_{a}^{1/2}. \tag{9}$$

As shown in Rodgers (2000), the singular vectors of this scaled weighting function matrix $\tilde{\mathbf{K}}$ represent independent vertical profiles that can be measured with the set of observations. The respective singular values are a direct measure of the signal-to-noise ratio taking into account our prior knowledge of the atmospheric state. Thus, singular vectors with a singular value larger than 1 contain usable information about the atmospheric state, and singular vectors with a singular value smaller than 1 are dominated by the measurement noise. Rodgers (2000) also shows that we can use these singular values to calculate the degrees of freedom for signal

$$d_s = \sum_i \frac{\lambda_i^2}{(1 + \lambda_i^2)} \tag{10}$$

and the information content

$$H = \frac{1}{2} \sum_{i} \ln(1 + \lambda_i^2). \tag{11}$$

Therefore, by calculating the singular values of K we have three measures of information for a certain set of observations considering our prior knowledge: (i) the number of independent measurements made to better than measurement error, (ii) the degrees of freedom for each independent measurement and the total degrees of freedom for the set of observations, and (iii) the Shannon information content of each independent measurement and the total Shannon information content for the set of observations. In the next section, we will also consider the estimated error in the retrieved columnaveraged volume mixing ratio, which can be calculated from the retrieval error covariance matrix \mathbf{S}_x as follows (Rodgers and Connor 2003).

$$\sigma^2 = \mathbf{g}^{\mathsf{T}} \mathbf{S} \mathbf{g},\tag{12}$$

where \mathbf{g} is an operator that converts the level volume mixing ratios to a column-averaged mixing ratio:

$$\mathbf{g} = \frac{\Delta p_i}{\sum_i \Delta p_i},\tag{13}$$

where Δp_i is the pressure thickness of layer i.

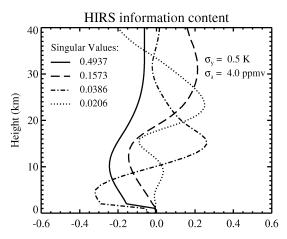
3. Application to HIRS and AIRS observing systems

Using the above-described theory, we calculated the information content with respect to atmospheric CO₂ for observations by TOVS/HIRS and AIRS. We used a broadband Malkmus radiative transfer model to calculate the weighting functions (Engelen et al. 2001). For AIRS, we used a spectral resolution of 1 cm⁻¹ for the band between 500 and 2500 cm⁻¹; for HIRS we used the spectral channels sensitive to CO₂ defined by the half-width of the instrumental response functions, which is about 15 cm⁻¹ for the longwave channels and about 25 cm⁻¹ for the shortwave channels. The channels used were channels 1-7 and 15-17 (Smith et al. 1979). The measurement covariance matrix for both instruments was specified as a diagonal matrix with standard deviations of 0.5 K on the diagonal elements. This error includes uncertainties in the temperature profile, which acts in this simple setup as an input for the radiative transfer model. These temperatures could come from the Advanced Microwave Sounding Unit or a weather forecast model. The above assumptions for the measurement covariance matrix are optimistic, especially because errors in the assumed temperature profiles will introduce correlations. Also, the value of 0.5 K is small. Therefore, we will also use a value of 1.0 K in one of the experiments. The a priori covariance matrix has, in our first example, diagonal elements of 16 (ppmv)² (standard deviation of 4 ppmv) and off-diagonal elements specified as follows:

$$S_{ij} = \sigma_a^2 \exp(-|z_i - z_j|/H),$$
 (14)

where the linear-scale height H is set to 25 km and where the minimum vertical correlation is set to 0.5. The lowest 2 km, which represents the boundary layer, was decoupled from the rest of the atmosphere by setting the correlations to zero. This covariance matrix setup, including the uncertainty estimate of 4 ppmv, was based on hourly output of CO_2 profiles from a GCM simulation (S. Denning, Colorado State University, 2002, personal communication). Although the uncertainty at individual levels is 4 ppmv, the uncertainty in the column-averaged mixing ratio is 3.1 ppmv [using (12)] because of the correlations between the levels.

Figure 1 shows the singular vectors and their corresponding singular values for both HIRS and AIRS with an a priori standard deviation of 4 ppmv. Only singular values that are larger than 1 are significant with respect to the measurement error. HIRS has no significant vectors; AIRS has two significant vectors. The first two AIRS singular vectors represent broad vertical patterns without much vertical resolution. The third AIRS singular vector adds some vertical resolution but is not significant. The degrees of freedom and the Shannon information content for this setup are shown in Table 2. The total degrees of freedom for HIRS are only 0.22. The total Shannon information content is 0.18, which



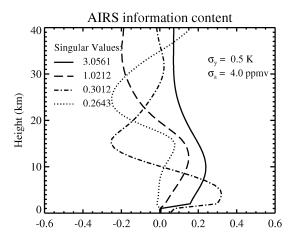


Fig. 1. First four singular vectors with their corresponding singular values for (left) HIRS and (right) AIRS. Measurement error was set to 0.5 K, and a priori error was set to 4 ppmv.

means that only $2^{0.18} = 1.1$ different atmospheric states can be detected. This means that within the a priori uncertainty of 4 ppmv less than two different atmospheric states can be distinguished. For AIRS, however, the total degrees of freedom is 1.6 and the total Shannon information content is 2.3, which translates into five distinguishable atmospheric states within the a priori uncertainty. The retrieval error of the column-averaged mixing ratio is 2.8 ppmv for HIRS and 1.2 ppmv for AIRS. There is some CO₂ signal in the HIRS radiances, but it is clearly not enough to observe atmospheric CO₂ concentrations at better than 4 ppmv. On the other hand, radiances observed by AIRS will be capable of providing significant atmospheric CO₂ information, especially total column values, as is shown by the first two singular vectors. What is also interesting to note is that the singular vectors for HIRS and AIRS are very similar. It is apparent that there is not a great difference in what structures both instruments can observe; the difference is in the signal-to-noise ratio reflected by the information content.

If we increase our a priori uncertainty to 10 ppmv (with a column-averaged uncertainty of 7.6 ppmv), which is close to the seasonal amplitude of atmospheric CO₂ concentrations, the HIRS radiances have a clearer signal, as shown in Table 3. The singular vectors are

Table 2. Singular values and the contribution of each singular vector to the degrees of freedom and information content for HIRS and AIRS with a priori CO_2 errors of 4 ppmv and observation errors of 0.5 K. The total degrees of freedom and the total information content are shown in the bottom row.

		HIRS			AIRS	
i	λ_i	d_s	Н	λ_i	d_s	Н
1	0.4937	0.1960	0.1573	3.0561	0.9033	1.6850
2	0.1573	0.0242	0.0176	1.0212	0.5105	0.5153
3	0.0386	0.0015	0.0011	0.2643	0.0653	0.0487
4	0.0206	0.0004	0.0003	0.2643	0.0653	0.0487
Total		0.2220	0.1763		1.5677	2.3157

the same as in Fig. 1, but the singular values (and therefore the degrees of freedom) and the Shannon information content have changed. HIRS now has one significant singular vector, and the degrees of freedom have increased to almost 1. The total Shannon information content is now 0.78, which represents almost two different atmospheric states. This means that HIRS is able to estimate a column-averaged CO2 concentration as represented by the first singular vector when our prior knowledge is on the order of 10 ppmv. AIRS still has two significant singular vectors. The total number of atmospheric states that can be detected by AIRS has increased to 32. The column-averaged retrieval errors are now 5.1 ppmv for HIRS and 2.2 ppmv for AIRS. This result shows that AIRS can significantly improve over the a priori estimate but HIRS does not reach an uncertainty that would be small enough to have a significant effect in CO₂ inversions.

Our estimate of the effect of errors in the assumed temperature profile on the forward radiative transfer model is conservative. We assumed an error of 0.5 K, but it could easily be as large as 1–2 K. Table 4 shows the retrieval statistics for an a priori error of 4 ppmv and a total measurement and forward model error of 1 K for both HIRS and AIRS. As before, HIRS does not have any significant singular values and its degrees of freedom dropped to 0.06 with 1.0 distinguishable atmospheric state. The retrieval error of the column-av-

Table 3. The same as in Table 2 but with a priori CO_2 errors of 10 ppmv and observation errors of 0.5 K.

	HIRS			AIRS			
i	λ_i	d_s	Н	λ_i	d_s	Н	
1 2 3 4 Total	1.2342 0.3933 0.0964 0.0516	0.6037 0.1339 0.0092 0.0027 0.7496	0.6676 0.1037 0.0067 0.0019 0.7800	7.6401 2.5531 0.7529 0.6606	0.9832 0.8670 0.3618 0.3038 2.5496	2.9459 1.4552 0.3240 0.2612 5.0109	

TABLE 4. The same as in Table 2 but with a priori CO₂ errors of 4 ppmv and observation errors of 1 K.

	HIRS			AIRS			
i	λ_i	d_s	Н	λ_i	d_s	Н	
1	0.2468	0.0574	0.0427	1.5280	0.7001	0.8688	
2	0.0787	0.0062	0.0045	0.5106	0.2068	0.1671	
3	0.0193	0.0004	0.0003	0.1506	0.0222	0.0162	
4	0.0103	0.0001	0.0001	0.1321	0.0172	0.0125	
Total		0.0641	0.0408		0.9477	1.0657	

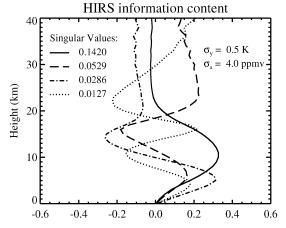
TABLE 5. The same as in Table 2 but for a diagonal a priori covariance matrix without any vertical correlations.

		HIRS			AIRS	
i	λ_i	d_s	Н	λ_{i}	d_s	Н
1	0.1420	0.0198	0.0144	0.8497	0.4193	0.3921
2	0.0529	0.0028	0.0020	0.3360	0.1014	0.0772
3	0.0286	0.0008	0.0006	0.2260	0.0486	0.0359
4	0.0127	0.0002	0.0001	0.1425	0.0199	0.0145
Total		0.0236	0.0171		0.5983	0.5262

eraged volume mixing ratio is 3.0 ppmv. The AIRS retrievals also degrade, but there is still one significant singular value. The total degrees of freedom is now 0.95, and the number of distinguishable atmospheric states is 2.1. The retrieval error of the column-averaged volume mixing ratio is 1.8 ppmv. For the case with a 10-ppmv a priori error specification, similar degradation results are obtained.

Although our specification of the a priori covariance matrix is an estimate based on model output, we now show the role of well-specified vertical correlations in the covariance matrix. Figure 2 and Table 5 show the results of the first experiment, but now with a diagonal a priori covariance matrix that contains no vertical correlations at all. Because the levels are completely uncorrelated, errors at different levels start to compensate when we calculate the column-averaged uncertainty. This column-averaged uncertainty of the a priori diagonal covariance matrix here specified is 0.98 ppmv. Both HIRS and AIRS show singular vectors with more vertical structure, but the singular values have decreased significantly. HIRS does not have any significant singular vectors at all, and the number of significant singular vectors for AIRS is also reduced to zero. The number of distinguishable atmospheric states is now 1.0 for HIRS and 1.4 for AIRS. The column-averaged uncertainty for HIRS is 0.97 ppmv, which is basically equal to the a priori uncertainty. The column-averaged uncertainty for AIRS is 0.87 ppmv. So, although the nondiagonal a priori covariance matrix seems to constrain the retrieval more than the diagonal a priori covariance matrix, the amount of information that can be retrieved from the observations is actually higher for the nondiagonal matrix. The reason for this result is that the weighting functions see only large-scale structure. The nondiagonal covariance matrix constrains the small-scale structure but has a larger variance at the larger scale, therefore allowing retrieval of more information about the large-scale structure than does the pure diagonal covariance matrix.

All analyses in this section have been carried out for individual profiles. However, to reduce the retrieval error, spatial and temporal averaging could be applied so as to render CO₂ distributions on spatial and temporal scales that are useful for current inversion studies. Most recent CO₂ inversion studies have used monthly mean observations and a transport model grid on the order of 5°-10° (e.g., Gurney et al. 2002; Kaminski et al. 2002; Rödenbeck et al. 2003). Most areas with significant cloudiness would allow the averaging of at least several satellite observations on these space and time scales. However, although averaging will reduce the random component of the observation error, any systematic errors in the retrieved values will remain in the averaged product. These systematic errors arise from biases in the a priori estimates, biases in the radiative transfer modeling, and biases in the temperature field. Furthermore, most of these biases are spatially heterogeneous, which



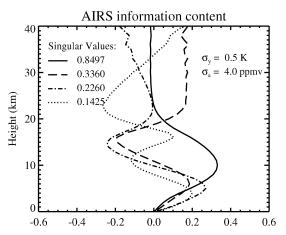


FIG. 2. Same as in Fig. 1, but now with a diagonal a priori covariance matrix (no vertical correlations).

will create errors in the horizontal gradients of the averaged CO₂ fields. Therefore, a proper characterization of especially these systematic errors is crucial for a correct interpretation of the results.

4. Summary

One of the important advantages of the higher-resolution sounders planned in the National Polar Orbiter Environmental Satellite System (NPOESS) and European Meteorological Operational Polar-Orbiting Satellite (METOP) era is the possibility for extracting nontraditional information from the measurements they provide. It is within this context that we describe the extent to which CO₂ may be directly retrieved from AIRS radiance data or data from similar emission-based spectrometer systems using information content theory. The analyses presented in this paper are also contrasted with the same analyses applied to TOVS/HIRS.

We have shown that the retrieval of CO₂ column concentrations from high-spectral-resolution infrared sounders looks promising, confirming the earlier results of Engelen et al. (2001). These retrievals potentially offer high enough accuracy to be useful for CO2 inversion studies that seek to estimate sinks and sources, although the information is concentrated mainly in the free troposphere and only very broad structures can be observed. This result suggests that weighted free tropospheric column retrieval is feasible. On the other hand, the current TOVS/HIRS instrument is only able to detect signals comparable to the seasonal amplitude of atmospheric CO₂. Both instruments could benefit from spatial and temporal averaging of the individual retrievals, but any systematic error would be retained in the averaged CO₂ values, which could lead to errors in the spatial gradients of the CO2 fields. The use of the existing 23-yr record of HIRS observations is probably of limited use for inversion studies, but the data might be very useful to get a long-term observational view of the seasonal atmospheric CO₂ variability. Specifying a correct a priori covariance matrix is very important to obtain the most information from the observations. Small-scale vertical structures should be constrained more strongly than large-scale vertical structures because the weighting functions are generally broad and the retrieval can therefore only retrieve information about the large-scale structures.

Plans exist to augment the data obtained by the highresolution sounders with data from spectrometers designed to measure the spectrally reflected sunlight at ultrafine resolution in specific CO₂ absorption bands. The CO₂ measurement approach using these measurements is described in O'Brien and Rayner (2002) and employs radiance measurements in two carefully selected absorption bands located in the near-infrared region of the solar spectrum. The complementary nature of these observations and the extent to which they add information on boundary layer CO₂ are currently under investigation.

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